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Quantum Surface of Section Method: Eigenstates and Unitary Quantum Poincaré Evolution

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Abstract The *unitary* representation of *exact* quantum Poincaré mapping is constructed. It is equivalent to the *compact* representation [19, 22, 23] in a sense that it yields equivalent quantization condition with important advantage over the compact version: since it preserves the probability it can be literally interpreted as the quantum Poincaré mapping which generates quantum time evolution at fixed energy between two successive crossings with surface of section (SOS). SOS coherent state representation (SOS Husimi distribution) of arbitrary (either stationary or evolving) quantum SOS state (vector from the Hilbert space over the configurational SOS) is introduced. Dynamical properties of SOS states can be quantitatively studied in terms of the so called localization areas which are defined through information entropies of their SOS coherent state representations. In the second part of the paper I report on results of extensive numerical application of quantum SOS method in a generic but simple 2-dim Hamiltonian system, namely semiseparable oscillator. I have calculated the stretch of 13 500 consecutive eigenstates with the largest sequential quantum number around 18 million and obtained the following results: (i) the validity of the semiclassical Berry-Robnik formula for level spacing statistics was confirmed and using the concept of localization area the states were quantitatively classified as regular or chaotic, (ii) the classical and quantum Poincaré evolution were performed and compared, and expected agreement was found, (iii) I studied few examples of wavefunctions and particularly, SOS coherent state representation of regular and chaotic eigenstates and analyzed statistical properties of their zeros which were shown on the chaotic component of 2-dim SOS to be uniformly distributed with the cubic repulsion between nearest neighbours.

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1 Introduction

In recent papers [19, 22, 23] the author established the surface of section (SOS) reduction of quantum dynamics in complete analogy with the famous Poincaré SOS reduction of classical dynamics [16]. In a similar way, as the smooth bound autonomous classical Hamiltonian dynamics in $2f$-dim phase space can be reduced to a discrete area preserving (Poincaré) mapping over $2(f-1)$-dim SOS, the essential information about quantum dynamics is contained in the energy-dependent propagator which acts over the Hilbert space of complex valued functions over $(f-1)$-dim configurational surface of section (CSOS) — the so called quantum Poincaré mapping (QPM). One can prove [19, 22, 23] the following interesting results which constitute quantum SOS reduction: (i) the eigenenergies of the original bound Hamiltonian are the points where the QPM possesses "nontrivial" fixed points, (ii) there exist additional three energy-dependent propagators which propagate from/to L^2(CS) to/from L^2(CSOS) or L^2(CS) (interpreted as propagators at fixed energy and without crossing the CSOS) and decompose the energy-dependent quantum propagator $(E-\hat{H})^{-1}$ in terms of newly defined propagators with respect to CSOS. One can consistently write the QPM as the product of two generalized (non-unitary) multi-channel scattering operators which correspond to two scattering problems which are obtained by cutting one half of CS along CSOS off and attaching a semi-infinite flat waveguide instead, in such a way that the two scattering Hamiltonians remain continuous. Such *compact* QPM (since, in a language of functional analysis, it is a compact operator) is consistent with its semiclassical limit [23] derived by Bogomolny a few years ago [5]. The same form of QPM was proposed for exact quantization of billiards by Smilansky and coworkers [31, 11]. And quite recently, Rouvinez and Smilansky [30] used the same technique for the quantization of a smooth 2-dim Hamiltonian.

But this compact QPM has one important disadvantage: Since it is not norm-preserving i.e. nonunitary operator it cannot be used to define quantum SOS evolution in analogy with the classical time evolution generated by the classical Poincaré mapping. It is only approximately unitary (its eigenvalues typically lie in the neighbourhood of a complex unit circle) and becomes unitary only in the semiclassical limit [5]. It is the purpose of this paper to show that there exists another consistent, equivalent and unique quantum SOS reduction in which QPM is strictly unitary. Such QPM is norm-preserving and it may be used to define unique quantum SOS time evolution of quantum SOS states (vectors from L^2(CSOS)) which corresponds to classical SOS time evolution. Each quantum SOS state may be represented by a kind of quantum SOS probability distribution function which is defined as its coherent state representation — Husimi distribution in terms of suitably defined SOS coherent states. This SOS Husimi distribution (analogously one could define nonpositive SOS Wigner distribution) may be used to study localization properties of quantum SOS states and their correlation with classical invariant components of SOS. I define a quantitative measure of localization, the so called localization area of a quantum SOS state which is defined through the information entropy of the corresponding SOS Husimi distribution.

The second purpose of this paper is to demonstrate the practical power of the unitary quantum SOS method as applied to a geometrically special, simple but dynamically generic (nonlinear) autonomous Hamiltonian system, namely 2-dim semiseparable oscillator. Using SOS reduction of quantum dynamics we were able to calculate a stretch of 13 500 consecutive eigenenergies and eigenstates with the sequential quantum number around 18 million. We have chosen a generic regime where classical dynamics of a system is mixed with regular and chaotic regions coexisting in phase space and on SOS. Thus I

was able to review many phenomena and confirm several conjectures of quantum chaos: (i) I confirmed the validity of semiclassical Berry-Robnik formula [4] for the energy level spacing distribution and quantitatively classified the eigenstates as regular or chaotic by means of their localization areas, (ii) I have explicitly studied SOS time evolution of quantum and classical SOS probability distributions and found expected agreement within the so called break time, (iii) I have studied few special examples of wavefunctions of eigenstates in configuration space, (iv) and SOS Husimi distributions of eigenstates and analyzed the statistical properties of their zeros [2] and found that they are uniformly distributed over the chaotic component of SOS with the cubic repulsion between nearest neighbours while in regular region they typically condense close to 1-dim classically invariant or anti-Stokes [17] curves. This confirms and extends the conjecture by Leboeuf and Voros [17].

2 Unitary Quantum Surface of Section Method

First we shall review some of the already known basic results [23] of the quantum SOS method which will be needed for further derivation of its unitarized version. We study *autonomous* and *bound* (at least in the energy region of our concern) Hamiltonian systems with few, say f, freedoms, living in an $f-$dim *configuration space* (CS) $\mathcal{C}$. One should also provide a smooth orientable $(f-1)$-dim submanifold of CS $\mathcal{C}$ which shall be called *configurational surface of section* (CSOS) and denoted by $\mathcal{S}_0$. CSOS $\mathcal{S}_0$ cuts the CS $\mathcal{C}$ in two pieces which will be referred to as upper and lower and denoted by $\mathcal{C}_\sigma$ with two values of the binary index $\sigma =\uparrow,\downarrow$. The two parts of the boundary of $\mathcal{C}$ which lie above/below $\mathcal{S}_0$ will be denoted by $\mathcal{B}_\sigma$. If CS $\mathcal{C}$ is infinite then $\boldsymbol{q}\in\mathcal{B}_\sigma$ will stand for the limiting process $|\boldsymbol{q}|\to\infty$ with $\boldsymbol{q}\in\mathcal{C}_\sigma$. In arithmetic expressions the arrows will have the following values $\uparrow=+1,\downarrow=-1$. We choose the coordinates in CS, $\boldsymbol{q}=(\boldsymbol{x},y)\in\mathcal{C}$ in such a way that the CSOS is given by a simple constraint $y=0$, or $\mathcal{S}_0=(\mathcal{S},0)$. These coordinates *need not be global*, i.e. they need not uniquely cover the whole CS, but they should cover the open set which includes the whole CSOS $\mathcal{S}_0$. This means that every point in $\mathcal{S}_0$ should be uniquely represented by CSOS coordinates $\boldsymbol{x}\in\mathcal{S}$ which *may be more general* than Euclidean coordinates $\mathcal{R}^{f-1}$ (e.g. $(f-1)$ dim sphere S^{f-1}).

We shall assume that the Hamiltonian has the following quite general form

$$H=\frac{1}{2m}p_y^2+H'(\boldsymbol{p}_x,\boldsymbol{x},y), \tag{1}$$

so that the kinetic energy is quadratic at least perpendicularly to the CSOS. There is straightforward generalization of the theory to the cases of nonconstant but positionally dependent mass and slightly less straightforward generalization to the cases of external gauge fields where we have also terms which are linear in momentum p_y [23].

In quantum mechanics, the observables are represented by self-adjoint operators in a Hilbert space $\mathcal{H}$ of complex-valued functions $\Psi(\boldsymbol{q})$ over the CS $\mathcal{C}$ which obey boundary conditions $\Psi(\partial\mathcal{C})=0$ and have finite L^2 norm $\int_{\mathcal{C}}d\boldsymbol{q}|\Psi(\boldsymbol{q})|^2<\infty$. We shall use the Dirac's notation. Pure state of a physical system is represented by a vector — *ket* $|\Psi\rangle$ which can be expanded in a convenient complete set of basis vectors, e.g. position eigenvectors $|\boldsymbol{q}\rangle=|\boldsymbol{x},y\rangle$, $|\Psi\rangle=\int_{\mathcal{C}}d\boldsymbol{q}|\boldsymbol{q}\rangle\langle\boldsymbol{q}|\Psi\rangle=\int_{\mathcal{C}}d\boldsymbol{q}\Psi(\boldsymbol{q})|\boldsymbol{q}\rangle$ (in a symbolic sense, since $|\boldsymbol{q}\rangle$ are not proper vectors, but such expansions are still meaningful iff $\Psi(\boldsymbol{q})=\langle\boldsymbol{q}|\Psi\rangle$ is square

[2] They exist since SOS Husimi function may be written according to Bargmann [2] in terms of analytic functions of $(f-1)$ complex variables.

integrable i.e. $L^2(\mathcal{C})$-function). Every ket $|\Psi\rangle \in \mathcal{H}$ has a corresponding vector from the dual Hilbert space $\mathcal{H}'$, that is *bra* $\langle\Psi| \in \mathcal{H}'$, $\langle\Psi|\boldsymbol{q}\rangle = \langle\boldsymbol{q}|\Psi\rangle^*$. We shall use mathematical accent $\hat{}$ to denote linear operators over the Hilbert space $\mathcal{H}$. An operator $\hat{A}$ acts either on abstract ket or on the corresponding wavefunction $\hat{A}\Psi(\boldsymbol{q}) = \langle\boldsymbol{q}|\hat{A}|\Psi\rangle$. The major problem of bound quantum dynamics governed by the self-adjoint Hamiltonian $\hat{H}$ is to determine the *eigenenergies* E for which the *Schrödinger equation*

$$\hat{H}\Psi_\sigma(\boldsymbol{q}, E) = E\Psi_\sigma(\boldsymbol{q}, E) \tag{2}$$

has nontrivial normalizable solutions — *eigenfunctions* $\Psi(\boldsymbol{q}, E)$.

Operators of SOS coordinates $\hat{\boldsymbol{x}}$ and $\hat{\boldsymbol{p}}_{\boldsymbol{x}}$, defined by

$$\begin{aligned} \langle\boldsymbol{x}, y|\hat{\boldsymbol{x}}|\Psi\rangle &= \boldsymbol{x}\Psi(\boldsymbol{x}, y), \\ \langle\boldsymbol{x}, y|\hat{\boldsymbol{p}}_{\boldsymbol{x}}|\Psi\rangle &= -i\hbar\partial_{\boldsymbol{x}}\Psi(\boldsymbol{x}, y), \end{aligned}$$

can be viewed also as acting on functions $\psi(\boldsymbol{x})$ of $\boldsymbol{x}$ only and therefore operating in some other, much smaller Hilbert space of square-integrable complex-valued functions over a CSOS $\mathcal{S}_0$

$$\begin{aligned} \{\boldsymbol{x}|\check{\boldsymbol{x}}|\psi\} &= \boldsymbol{x}\psi(\boldsymbol{x}), \\ \{\boldsymbol{x}|\check{\boldsymbol{p}}_{\boldsymbol{x}}|\psi\} &= -i\hbar\partial_{\boldsymbol{x}}\psi(\boldsymbol{x}). \end{aligned}$$

Vectors in such reduced SOS Hilbert space, denoted by $\mathcal{L}$, will be written as $|\psi\}$ and linear operators over $\mathcal{L}$ will wear mathematical accent $\check{}$ like restricted position $\check{\boldsymbol{x}}$ and momentum $\check{\boldsymbol{p}}_{\boldsymbol{x}}$. Eigenvectors $|\boldsymbol{x}\}$ of SOS position operator $\check{\boldsymbol{x}}$ provide a useful complete set of basis vectors of $\mathcal{L}$. The quantum Hamiltonian can be written in position representation at least locally as

$$\hat{H} = -\frac{\hbar^2}{2m}\partial_y^2 + \hat{H}'(y), \quad \hat{H}'(y) = H'(-i\hbar\partial_{\boldsymbol{x}}, \boldsymbol{x}, y). \tag{3}$$

The eigenstates of the *reduced Hamiltonian* $\check{H}'(0) = \hat{H}'(0)|_{\mathcal{L}}$ restricted to the SOS Hilbert space $\mathcal{L}$, $|n\} \in \mathcal{L}$

$$\check{H}'(0)|n\} = E'_n|n\}, \tag{4}$$

which are called *SOS eigenmodes*, provide a useful (countable $n = 1, 2, \ldots$) complete and orthogonal basis for $\mathcal{L}$ since $\check{H}'(0)$ is a self-adjoint operator with discrete spectrum when its domain is restricted to $\mathcal{L}$.

2.1 Scattering formulation of quantum SOS

In order to make the paper selfcontained we shall here review some crucial ingredients of a scattering formulation of quantum SOS method [20, 23, 30] which will be needed for further derivation of its unitarized version.

Let us consider for the moment an open quantum (quasi 1-dim) waveguide with the Hamiltonian

$$\hat{H}_{\text{free}} = \frac{\hat{p}_y^2}{2m} + H'(\hat{\boldsymbol{p}}_{\boldsymbol{x}}, \hat{\boldsymbol{x}}, 0) = -\frac{\hbar^2}{2m}\partial_y^2 + \hat{H}'(0). \tag{5}$$

The motion it describes is free in $y-$direction and bound in all other $\boldsymbol{x}$-directions. The basic solutions of the Schrödinger equation at some arbitrary energy E in such waveguide are separable to products of plane waves in $y-$ direction and SOS eigenmodes

in $\boldsymbol{x}-$direction $\{\boldsymbol{x}|n\}e^{\pm ik_n(E)y}$, with the corresponding wavenumber determined by the energy difference $E-E'_n$ available for the free motion perpendicular to the CSOS

$$k_n(E)=\sqrt{\frac{2m}{\hbar^2}(E-E'_n)}.$$

Such basic solutions for any n will be called *channels*, and there are typically finitely many *open* or *propagating* channels n for which the energy difference $E-E'_n$ is positive, that is the wavenumber $k_n(E)$ is positive real, and infinitely many *closed* or *evanescent* channels n for which the energy difference $E-E'_n$ is negative, which means that wavenumber $k_n(E)$ is positive imaginary. Sometimes I will write $\mathcal{L}_o(E)$ for the finitely dimensional subspace of $\mathcal{L}$ spanned by SOS eigenmodes corresponding to open channels and $\mathcal{L}_c(E)$ for its orthogonal complement, so that $\mathcal{L}=\mathcal{L}_o(E)\oplus\mathcal{L}_c(E)$. If one defines the wavenumber operator over $\mathcal{L}$

$$\check{K}(E)=\sum_n k_n(E)|n\}\{n|=\sqrt{\frac{2m}{\hbar^2}(E-\check{H}'(0))}. \tag{6}$$

then a general (nonbound) solution of the Schrödinger equation in the waveguide may be compactly written in terms of arbitrary two SOS states $|\vartheta_\uparrow\},|\vartheta_\downarrow\}\in\mathcal{L}$

$$\Psi(\boldsymbol{x},y,E)=\frac{\hbar}{\sqrt{-im}}\{\boldsymbol{x}|\check{K}^{-1/2}(E)\left[e^{i\check{K}(E)y}|\vartheta_\uparrow\}+e^{-i\check{K}(E)y}|\vartheta_\downarrow\}\right] \tag{7}$$

where the prefactors $\hbar(-imk_n)^{-1/2}$ in front of each component $\{n|\vartheta_\sigma\}$ provide convenient normalization. To connect bound Hamiltonian dynamics and scattering theory one should make the following very important step. Cut one part of CS off along CSOS ($y=0$) and attach a semi-infinite waveguide (5) instead. Thus we introduce two scattering Hamiltonians

$$\hat{H}_\sigma=\begin{cases}-(\hbar^2/2m)\partial_y^2+\hat{H}'(y); & \sigma y\geq 0,\\ -(\hbar^2/2m)\partial_y^2+\hat{H}'(0); & \sigma y<0.\end{cases} \tag{8}$$

Let $\Psi_\sigma(\boldsymbol{x},y,E)$ denote a scattering wavefunction which is a solution of the Schrödinger equation with the scattering Hamiltonian (8) while it is also the solution of the ordinary bound Schrödinger equation (2) on the $\sigma-$side $\mathcal{C}_\sigma$ ($\sigma y\geq 0$). In the waveguide ($\sigma y\leq 0$) any scattering wavefunction may be written in a form (7) where the two SOS states are no longer arbitrary but they are related through a generalized multichannel scattering operator $\check{T}_\sigma(E)\in\mathcal{L}$

$$|\vartheta_{-\sigma}\}=\check{T}_\sigma(E)|\vartheta_\sigma\} \tag{9}$$

since scattering wavefunction $\Psi_\sigma(\boldsymbol{x},y,E)$ should satisfy proper boundary conditions on the $\sigma-$side, $\Psi_\sigma(\boldsymbol{q}\in\mathcal{B}_\sigma,E)=0$.

Now one can easily give *necessary condition* for an energy E to be an eigenenergy of the original bound Hamiltonian $\hat{H}$. Then an eigenfunction $\Psi(\boldsymbol{x},y)$ should exist and the two scattering wavefunctions $\Psi_\sigma(\boldsymbol{x},y,E)$ with the following SOS representation inside the waveguide

$$\Psi_\sigma(\boldsymbol{x},y,E)=\frac{\hbar}{\sqrt{-im}}\{\boldsymbol{x}|\check{K}^{-1/2}(E)\left[e^{i\sigma\check{K}(E)y}+e^{-i\sigma\check{K}(E)y}\check{T}_\sigma(E)\right]|\vartheta_\sigma\} \tag{10}$$

and which match the eigenfunction outside the waveguide

$$\Psi(\boldsymbol{x},y)=\Psi_{\mathrm{sign}(y)}(\boldsymbol{x},y,E).$$

One should further require that eigenfunction $\Psi(\boldsymbol{x}, y)$ and its normal derivative $\partial_y \Psi(\boldsymbol{x}, y)$ written in terms of $\Psi_\sigma(\boldsymbol{x}, y, E)$ should be continuous on CSOS ($y = 0$) which results in two simple equations $(1 \pm \check{T}_\uparrow)|\vartheta_\uparrow\} = -(1 \pm \check{T}_\downarrow)|\vartheta_\downarrow\}$ which in turn are equivalent to the condition that $|\vartheta_\uparrow\}$ is a fixed point of an operator $\check{T}(E) = \check{T}_\downarrow(E)\check{T}_\uparrow(E)$

$$\check{T}(E)|\vartheta_\uparrow\} = |\vartheta_\uparrow\}. \tag{11}$$

Even stronger result can be proved [23]: singularity of $1 - \check{T}(E)$ is also sufficient quantization condition if an energy E is not equal to the threshold E'_n for opening of some new mode n, and in this case the dimension of null space of $E - \hat{H}$ is the same as dimension of null space of $1 - \check{T}(E)$.

The product of generalized scattering operators $\check{T}(E)$ may be interpreted as CSOS-CSOS propagator or QPM although it is not a unitary but a compact operator and only the open-open parts of scattering operators $\check{T}_\sigma(E)$ (consisting of matrix elements between open modes) are unitary matrices [23, 30]. It is convenient to define *wave operators* which map any SOS state $|\vartheta_\sigma\}$ to the corresponding scattering function outside the waveguide $\Psi_\sigma(\boldsymbol{x}, y, E)$ and vice versa

$$\begin{aligned} \langle \boldsymbol{x}, y|\acute{Q}_\sigma(E)|\vartheta_\sigma\} &= \theta(\sigma y)\Psi_\sigma(\boldsymbol{x}, y, E), & (12)\\ \{\vartheta^*_\sigma|\grave{P}_\sigma(E)|\boldsymbol{x}, y\rangle &= \theta(\sigma y)\Psi^*_\sigma(\boldsymbol{x}, y, E^*). & (13) \end{aligned}$$

($\theta(y)$ is the Heaviside step function) where the dual SOS state $\{\vartheta^*_\sigma|$, which is in general different from $\{\vartheta_\sigma|$, generates complex conjugated scattering wavefunction

$$\Psi^*_\sigma(\boldsymbol{x}, y, E^*) = \frac{\hbar}{\sqrt{-im}}\{\vartheta^*_\sigma|\left[e^{i\sigma\check{K}(E)y} + e^{-i\sigma\check{K}(E)y}\check{T}_\sigma(E)\right]\check{K}^{-1/2}(E)|\boldsymbol{x}\}.$$

The linear operators $\acute{Q}_\sigma(E)$ from $\mathcal{L}$ to $\mathcal{H}$ and $\grave{P}_\sigma(E)$ from $\mathcal{H}$ to $\mathcal{L}$ may be interpreted as the quantum CSOS-CS and CS-CSOS propagators, respectively. If E is an eigenenergy of the original bound Hamiltonian $\hat{H}$ and $|\vartheta_\uparrow\}$ is the associated fixed point of QPM $\check{T}(E)$ then the corresponding wavefunction can be calculated by means of CSOS-CS propagator

$$\Psi(\boldsymbol{x}, y) = \langle \boldsymbol{x}, y|\acute{Q}_{\mathrm{sign}(y)}|\vartheta_{\mathrm{sign}(y)}\} = \langle \boldsymbol{x}, y|\acute{Q}_\uparrow|\vartheta_\uparrow\} + \langle \boldsymbol{x}, y|\acute{Q}_\downarrow|\vartheta_\downarrow\}$$

where $|\vartheta_\downarrow\} := \check{T}_\uparrow(E)|\vartheta_\uparrow\}$. The position matrix elements of the energy-dependent quantum scattering propagators $\hat{G}_\sigma(E) = (E - \hat{H}_\sigma + i0)^{-1}$ will be written as $G_\sigma(\boldsymbol{q}, \boldsymbol{q}', E) = \langle \boldsymbol{q}|\hat{G}_\sigma(E)|\boldsymbol{q}'\rangle$. Then we consider another, hybrid representation of scattering Green functions $\check{G}_\sigma(y, y', E)$, which are operator valued distributions acting over reduced SOS Hilbert space $\mathcal{L}$ defined by

$$\{\boldsymbol{x}|\hat{G}_\sigma(y, y', E)|\boldsymbol{x}'\} = \langle \boldsymbol{x}, y|\hat{G}(E)|\boldsymbol{x}', y'\rangle.$$

The three newly defined quantum propagators can be expressed in terms of scattering resolvents [22, 23]

$$\begin{aligned} \check{T}_\sigma(E) &= \frac{i\hbar^2}{m}\check{K}^{1/2}(E)\check{G}_\sigma(0, 0, E)\check{K}^{1/2}(E) - 1,\\ \langle \boldsymbol{x}, y|\acute{Q}_\sigma(E) &= \frac{\hbar}{\sqrt{-im}}\theta(\sigma y)\{\boldsymbol{x}|\check{G}_\sigma(y, 0, E)\check{K}^{1/2}(E),\\ \grave{P}_\sigma(E)|\boldsymbol{x}, y\rangle &= \frac{\hbar}{\sqrt{-im}}\theta(\sigma y)\check{K}^{1/2}(E)\check{G}_\sigma(0, y, E)|\boldsymbol{x}\}, \end{aligned}$$

If one defines additional *conditional* CS-CS propagator (without crossing CSOS) $\hat{G}_0(E)$ as

$$\langle \boldsymbol{x}, y|\hat{G}_0(E)|\boldsymbol{x}', y'\rangle = \begin{cases} \langle \boldsymbol{x}, y|\hat{G}_\uparrow(E)|\boldsymbol{x}', y'\rangle; & y \geq 0,\ y' \geq 0, \\ \langle \boldsymbol{x}, y|\hat{G}_\downarrow(E)|\boldsymbol{x}', y'\rangle; & y \leq 0,\ y' \leq 0, \\ 0; & yy' < 0. \end{cases} \tag{14}$$

then the usual (*unconditional*) energy-dependent quantum CS-CS propagator $\hat{G}(E) = (E - \hat{H})^{-1}$ can be decomposed in terms of four newly defined (CS/CSOS)-(CS/CSOS) propagators

$$\begin{aligned} \hat{G}(E) = \hat{G}_0(E) \quad &+ \quad \sum_\sigma \acute{Q}_\sigma(E)(1 - \check{T}_{-\sigma}(E)\check{T}_\sigma(E))^{-1}\grave{P}_{-\sigma}(E) \\ &+ \quad \sum_\sigma \acute{Q}_\sigma(E)(1 - \check{T}_{-\sigma}(E)\check{T}_\sigma(E))^{-1}\check{T}_{-\sigma}(E)\grave{P}_\sigma(E). \end{aligned} \tag{15}$$

All poles of the propagator $\hat{G}(E)$ — eigenenergies of $\hat{H}$ come from singularities of the form $(1-\check{T}(E))^{-1}$ so the quantization condition (11) is indeed justified. One is tempted to expand the factors like $(1 - \check{T}(E))^{-1}$ into geometric series and give all the terms and factors a firm physical interpretation in terms of probability amplitudes for quantum SOS propagation [19, 23]. But there is serious difficulty since such sum would be manifestly divergent since the operators $\check{T}_{-\sigma}(E)\check{T}_\sigma(E)$ have in general also eigenvalues whose magnitude is (slightly) larger than one. Now we proceed to show that there exist another unique realization of quantum SOS propagators with unitary QPM and conditionally convergent expansion of decomposition formula.

2.2 Reactance operator formulation and unitarization

In this subsection we will unitarize the compact scattering operators $\check{T}_\sigma(E)$ in three steps: (i) We will express the compact CSOS-CSOS propagators $\check{T}_\sigma(E)$ as the Caley transformation of reactance operators [18]. (ii) These reactance matrices will be made *Hermitian* by a simple transformation which preserves their open-open part (and thus preserving also the semiquantal and semiclassical limit) while it rotates the phases of components referring to close modes by $\pi/4$. (iii) Finally, we shall define *unitary* CSOS-CSOS propagators as the Caley transformation of Hermitian reactance operators.

The solution of the Schrödinger equation (2) is unique in any range of CS and at any energy when all the boundary conditions are known. Take any $L^2(\mathcal{S}_0)$ function over CSOS $\varphi(\boldsymbol{x}) = \{\boldsymbol{x}|\boldsymbol{\varphi}\}$ and denote by $\Phi_\sigma(\boldsymbol{q}, E)$ its extension as the solution of the Schrödinger equation (2) on the $\sigma-$side $\mathcal{C}_\sigma$ of CS with the boundary conditions

$$\Phi_\sigma(\boldsymbol{x}, 0, E) = \varphi(\boldsymbol{x}), \quad \Phi_\sigma(\boldsymbol{q} \in \mathcal{B}_\sigma, E) = 0. \tag{16}$$

If on the other side of CS one assumes $\Phi_\sigma(\boldsymbol{q} \in \mathcal{C}_{-\sigma}) = 0$ this may be written as a linear relationship $\acute{W}_\sigma(E)$ from $\mathcal{L}$ to $\mathcal{H}$

$$|\Phi\rangle = \acute{W}_\sigma(E)|\varphi\}.$$

For any value of energy E there exist nontrivial solutions of the Schrödinger equation on both sides of CS $\Phi_\sigma(\boldsymbol{q}, E)$ which have given values on the CSOS $\varphi(\boldsymbol{x})$. The entire wavefunction $\Phi(\boldsymbol{q}, E) = \Phi_\uparrow(\boldsymbol{q}, E) + \Phi_\downarrow(\boldsymbol{q}, E)$ is thus continuous on CSOS $\mathcal{S}_0$ by construction. But only for special values of E, eigenenergies, there exists such $\varphi(\boldsymbol{x})$ that also the normal derivative of the wavefunction $\partial_y\Phi(\boldsymbol{x}, y, E)$ is continuous at $y = 0$ so

that $\Phi(\boldsymbol{q},E)$ becomes the eigenfunction — the solution of Schrödinger equation on entire CS $\mathcal{C}$. The quantization condition $\partial_y\Phi_\uparrow(\boldsymbol{x},0,E)=\partial_y\Phi_\downarrow(\boldsymbol{x},0,E)$ can be written as the singularity condition for the sum of operators over $\mathcal{L}$

$$(\check{A}_\uparrow(E)+\check{A}_\downarrow(E))|\varphi\}=0 \tag{17}$$

which are defined by

$$\{\boldsymbol{x}|\check{A}_\sigma(E)|\varphi\}=\sigma\partial_y\Phi_\sigma(\boldsymbol{x},0,E). \tag{18}$$

It is easy to see that the quantization conditions (11) and (17) are equivalent, that $|\varphi\}$ is related to $|\vartheta_\sigma\}$, $\check{A}_\sigma(E)$ are related to $\check{T}_\sigma(E)$, and $\acute{W}_\sigma(E)$ are related to $\acute{Q}_\sigma(E)$. From the scattering ansatz (10) we see that one should put

$$|\vartheta_\sigma\}=(1+\check{T}_\sigma(E))^{-1}\check{K}^{1/2}(E)|\varphi\} \tag{19}$$

since then the scattering wavefunction $\Psi_\sigma(\boldsymbol{q},E)$ becomes proportional to the wavefunction $\Phi_\sigma(\boldsymbol{q},E)$ on $\mathcal{C}_\sigma$. Differentiating (10) with respect to y at $y=0$ one further obtains

$$\check{A}_\sigma(E)=i\check{K}^{1/2}(E)(1-\check{T}_\sigma(E))(1+\check{T}_\sigma(E))^{-1}\check{K}^{1/2}(E) \tag{20}$$

according to definition (18). Moreover, $\acute{Q}_\sigma(E)|\vartheta_\sigma\}=\acute{W}_\sigma(E)|\varphi\}$, so

$$\acute{W}_\sigma(E)=\acute{Q}_\sigma(E)(1+\check{T}_\sigma(E))^{-1}\check{K}^{1/2}(E). \tag{21}$$

Relation (20) calls for introduction of *generalized (nonhermitian)* multichannel reactance operators [18]

$$\check{R}_\sigma(E)=\check{K}^{-1/2}(E)\check{A}_\sigma(E)\check{K}^{-1/2}(E) \tag{22}$$

in terms of which one can write the generalized scattering operators as a Caley transformation

$$\check{T}_\sigma(E)=(1+i\check{R}_\sigma(E))(1-i\check{R}_\sigma(E))^{-1} \tag{23}$$

But for real energy $E=E^*$ the operators $\check{A}_\sigma(E)$ are Hermitian. To see this one should transform surface integral over $\mathcal{S}_0$ to a volume integral over $\mathcal{C}_\sigma$

$$\begin{aligned}\{\varphi|\check{A}_\sigma(E)|\varphi'\}&=\sigma\int\limits_{\mathcal{S}}d\boldsymbol{x}\Phi^*_\sigma(\boldsymbol{x},0,E^*)\partial_y\Phi'_\sigma(\boldsymbol{x},0,E)=\\&=\int\limits_{\mathcal{C}_\sigma}d\boldsymbol{q}\left(\partial_y\Phi^*_\sigma(\boldsymbol{q},E^*)\partial_y\Phi'_\sigma(\boldsymbol{q},E)+\Phi^*_\sigma(\boldsymbol{q},E^*)\frac{2m}{\hbar^2}(\hat{H}'(y)-E)\Phi'_\sigma(\boldsymbol{q},E)\right).\end{aligned} \tag{24}$$

Note that the second term of (24) is also symmetric since $\hat{H}'(y)$ does not involve derivative ∂_y. The operator $\check{K}^{1/2}(E)$ and therefore the reactance operators $\check{R}_\sigma(E)$ are nonhermitian since the square roots of wavenumbers are not all real due to existence of closed channels. But there is an easy an unique way (up to trivial constant similarity transformation) of how to make operator $\check{K}^{1/2}(E)$ Hermitian without touching the components referring to open modes $\mathcal{L}_o(E)$ which govern the physics in classically allowed regions of phase space. Let us define an operator

$$\check{\mathcal{K}}(E)=\sum_n\sqrt{\frac{2m}{\hbar^2}(E-E'_n)\mathrm{sign}(\mathrm{Re}E-E'_n)}|n\}\{n| \tag{25}$$

which is a Hermitian for real energy E while it may be analytically continued for complex E for $\mathrm{Re}E \neq E'_n$. Its square root may be conveniently written in terms of simple piecewise constant unitary transformation $\check{\mathcal{K}}^{1/2}(E) = \check{u}(E)\check{K}^{1/2}(E)$,

$$\check{u}(E) = \sum_n^{\mathrm{Re}E>E'_n} |n\}\{n| + \sum_n^{\mathrm{Re}E<E'_n} \sqrt{i}\,\mathrm{sign}(\mathrm{Im}E - 0)|n\}\{n|. \tag{26}$$

We always consider the branch of square root with positive real part. We shall usually omit energy dependence of operator $\check{u}$ since it is constant inside a given semiband $E'_n < \mathrm{Re}E < E'_{n+1}, \pm\mathrm{Im}E > 0$. Now one can define Hermitian reactance operators in analogy with (22)

$$\check{\mathcal{R}}_\sigma(E) = \check{\mathcal{K}}^{-1/2}(E)\check{A}_\sigma(E)\check{\mathcal{K}}^{-1/2}(E) = \check{u}^{-1}\check{R}_\sigma(E)\check{u}^{-1} \tag{27}$$

and in analogy with (23) one can define *unitary* operators

$$\check{\mathcal{T}}_\sigma(E) = (1 + i\check{\mathcal{R}}_\sigma(E))(1 - i\check{\mathcal{R}}_\sigma(E))^{-1}. \tag{28}$$

Unitary operators $\check{\mathcal{T}}_\sigma(E)$ are no longer proper scattering operators of scattering systems (8) but they may be called *unitarized scattering operators*. The quantization condition for original Hamiltonian $\hat{H}$ (17) may be restated as the singularity condition for the sum of Hermitian reactance matrices $\check{\mathcal{R}}(E) = \check{\mathcal{R}}_\uparrow(E) + \check{\mathcal{R}}_\downarrow(E)$

$$\check{\mathcal{R}}(E)|\rho\} = 0, \tag{29}$$

with (17,27)

$$|\rho\} = \check{\mathcal{K}}^{1/2}(E)|\varphi\}. \tag{30}$$

Equivalently, this can be written as a fixed point (eigenvalue 1) condition for the product of unitarized scattering propagators $\check{\mathcal{T}}(E) = \check{\mathcal{T}}_\downarrow(E)\check{\mathcal{T}}_\uparrow(E)$

$$\check{\mathcal{T}}(E)|\psi_\uparrow\} = |\psi_\uparrow\} \tag{31}$$

since one can use the definition (28) to derive a relation which connects (29) and (31)

$$1 - \check{\mathcal{T}}(E) = \frac{1}{2i}(1 + \check{\mathcal{T}}_\downarrow(E))\check{\mathcal{R}}_\sigma(E)(1 + \check{\mathcal{T}}_\uparrow(E))$$

and the two types of stationary SOS states are related by

$$|\rho\} = |\psi_\uparrow\} + |\psi_\downarrow\}, \quad |\psi_\sigma\} = (1 + \check{\mathcal{T}}_\sigma(E))^{-1}|\rho\} \tag{32}$$

where we have defined $|\psi_\downarrow\} := \check{\mathcal{T}}_\uparrow(E)|\psi_\uparrow\}$ so that general relation analogous to (9) holds

$$|\psi_{-\sigma}\} = \check{\mathcal{T}}_\sigma(E)|\psi_\sigma\}.$$

The fixed points of compact and unitary QPM are related by the formula

$$|\vartheta_\sigma\} = \left[\check{u} - \tfrac{1}{2}(\check{u} - \check{u}^{-1})(1 + \check{\mathcal{T}}_\sigma(E))\right]|\psi_\sigma\}.$$

which follows from eqs. (19,30,32).

2.3 Unitarized decomposition formula and interpretation

Now we show that we can interpret the operator $\check{\mathcal{T}}(E)$ as CSOS-CSOS propagator or QPM which has all desirable properties. One can define also the unitarized versions of other three conditional CS/CSOS-CS/CSOS propagators

$$\begin{aligned}
\acute{\mathcal{Q}}_\sigma(E) &= \acute{Q}_\sigma(E)\left[\breve{u} - \tfrac{1}{2}(\breve{u}-\breve{u}^{-1})(1+\check{\mathcal{T}}_\sigma(E))\right] \\
\grave{\mathcal{P}}_\sigma(E) &= \left[\breve{u} - \tfrac{1}{2}(1+\check{\mathcal{T}}_\sigma(E))(\breve{u}-\breve{u}^{-1})\right]\grave{P}_\sigma(E) \\
\hat{\mathcal{G}}_0(E) &= \hat{G}_0(E) + \frac{i}{4}\sum_\sigma \acute{Q}_\sigma(E)\left[1-\breve{u}^2 - \tfrac{1}{4}(\breve{u}-\breve{u}^{-1})(1+\check{\mathcal{T}}_\sigma(E))(\breve{u}-\breve{u}^{-1})\right]\grave{P}_\sigma(E)
\end{aligned} \tag{33}$$

and show by simple algebraic manipulation that the *unitarized decomposition formula* for energy-dependent quantum CS-CS propagator follows from (15)

$$\begin{aligned}
\hat{G}(E) = \hat{\mathcal{G}}_0(E) &+ \sum_\sigma \acute{\mathcal{Q}}_\sigma(E)(1-\check{\mathcal{T}}_{-\sigma}(E)\check{\mathcal{T}}_\sigma(E))^{-1}\grave{\mathcal{P}}_{-\sigma}(E) \\
&+ \sum_\sigma \acute{\mathcal{Q}}_\sigma(E)(1-\check{\mathcal{T}}_{-\sigma}(E)\check{\mathcal{T}}_\sigma(E))^{-1}\check{\mathcal{T}}_{-\sigma}(E)\grave{\mathcal{P}}_\sigma(E).
\end{aligned} \tag{34}$$

In definitions (33) we have multiplied by simple linear combinations of unitary operators so we have not introduced any singularities for real E. All poles of the resolvent $\hat{G}(E)$ again come from singularities of $(1-\check{\mathcal{T}}(E))^{-1}$ in accordance with (31). If $|\psi_\uparrow\}$ is a fixed point of $\check{\mathcal{T}}(E)$ for such an eigenenergy E then the corresponding wavefunction is given by

$$\Psi(\boldsymbol{x},y) = \langle \boldsymbol{x},y|\acute{\mathcal{Q}}_{\mathrm{sign}(y)}|\psi_{\mathrm{sign}(y)}\} = \langle \boldsymbol{x},y|\acute{\mathcal{Q}}_\uparrow(E)|\psi_\uparrow\} + \langle \boldsymbol{x},y|\acute{\mathcal{Q}}_\downarrow(E)|\psi_\downarrow\},$$

where $|\psi_\downarrow\} := \check{\mathcal{T}}_\uparrow(E)|\psi_\uparrow\}$. One can expand the factors $(1-\check{\mathcal{T}}(E))^{-1}$ in unitary decomposition formula in a geometric series

$$\hat{G}(E) = \sum_{n=0}^{\infty}\check{\mathcal{G}}_n(E), \tag{35}$$

with

$$\check{\mathcal{G}}_{2l+1}(E) = \sum_\sigma \acute{\mathcal{Q}}_\sigma(E)\left(\check{\mathcal{T}}_{-\sigma}(E)\check{\mathcal{T}}_\sigma(E)\right)^l\check{\mathcal{T}}_{-\sigma}(E)\grave{\mathcal{P}}_\sigma(E), \tag{36}$$

$$\check{\mathcal{G}}_{2l}(E) = \sum_\sigma \acute{\mathcal{Q}}_\sigma(E)\left(\check{\mathcal{T}}_{-\sigma}(E)\check{\mathcal{T}}_\sigma(E)\right)^l\grave{\mathcal{P}}_{-\sigma}(E), \quad l=0,1,2\ldots \tag{37}$$

This decomposition formula may be given the following firm physical interpretation. The quantum probability amplitude $\langle \boldsymbol{q}|\hat{G}(E)|\boldsymbol{q}'\rangle$ to propagate from point $\boldsymbol{q}'$ to point $\boldsymbol{q}$ in CS at energy E may be written as a sum of conditional probability amplitudes $\langle \boldsymbol{q}|\hat{\mathcal{G}}_l(E)|\boldsymbol{q}'\rangle$ to propagate from $\boldsymbol{q}'$ to $\boldsymbol{q}$ at energy E and cross CSOS exactly l times (35). If points $\boldsymbol{q}$ and $\boldsymbol{q}'$ lie on the same/opposite side of CS with respect to CSOS then each continuous orbit must cross CSOS even/odd number of times and thus all probability amplitudes $\langle \boldsymbol{q}|\hat{\mathcal{G}}_l(E)|\boldsymbol{q}'\rangle$ for odd/even l are zero. Each probability amplitude $\langle \boldsymbol{q}|\hat{\mathcal{G}}_l(E)|\boldsymbol{q}'\rangle$ may be further decomposed as a sum of products of probability amplitudes by inserting an identity $\int d\boldsymbol{x}|\boldsymbol{x}\}\{\boldsymbol{x}|$ between each pair of factors in (36,37). The elementary propagators should be interpreted as follows: $\langle \boldsymbol{q}|\acute{\mathcal{Q}}_\sigma(E)|\boldsymbol{x}'\}, \{\boldsymbol{x}|\grave{\mathcal{P}}_\sigma(E)|\boldsymbol{q}'\rangle, \{\boldsymbol{x}|\check{\mathcal{T}}_\sigma(E)|\boldsymbol{x}'\}$ are conditional quantum probability amplitudes for a system to propagate at fixed energy E through $\sigma-$ side of CS $\mathcal{C}_\sigma$ from point $\boldsymbol{q}'$ in CS or point $\boldsymbol{x}'$ on CSOS to point $\boldsymbol{q}$ in CS or point $\boldsymbol{x}$ on CSOS and without crossing CSOS in between.

Each orbit of a bound system which crosses CSOS must cross it again with probability one, consistently with unitarity of CSOS-CSOS propagators

$$\int d\boldsymbol{x}|\{\boldsymbol{x}|\check{\mathcal{T}}_\sigma(E)|\boldsymbol{x}'\}|^2 = 1.$$

2.4 Quantum Poincaré evolution

Let us choose normalized initial SOS state $|0,\uparrow\}$. $\{\boldsymbol{x}|0,\uparrow\}$ should be interpreted as quantum probability amplitude that system's orbit initially crosses CSOS at $\boldsymbol{x}$ from below. Like for classical Poincaré evolution one should also specify the value of energy E besides CSOS coordinates $\boldsymbol{x}$ to completely determine system's dynamics. Then quantum Poincaré evolution is a simple iteration of unitary QPM $\check{\mathcal{T}}(E)$

$$|n+1,\uparrow\} = \check{\mathcal{T}}(E)|n,\uparrow\}. \tag{38}$$

When the system crosses CSOS n-th time from below, $\{\boldsymbol{x}|n,\uparrow\} = \{\boldsymbol{x}|\check{\mathcal{T}}^n(E)|0,\uparrow\}$ is a probability amplitude that it crosses CSOS at $\boldsymbol{x}$ if it was initially in a state $|0,\uparrow\}$. Existence of a stationary state implies existence of a fixed point of QPM $\check{\mathcal{T}}(E)$ which does not evolve, not even its phase.

Résumé: I have shown that the f-dim autonomous bound Hamiltonian quantum dynamics governed by a continuous group of unitary propagators $\{\exp(-it\hat{H}/\hbar); t \in \mathcal{R}\}$ is equivalent to a continuous family (labeled by energy) of $(f-1)$-dim discrete quantum systems governed by discrete groups of unitary propagators $\{\check{\mathcal{T}}^n(E); n = 0, \pm 1, \pm 2 \ldots\}$ just like the classical autonomous bound Hamiltonian dynamics with f freedoms is equivalent to a continuous family (labeled by energy) of discrete area preserving classical Poincaré mappings with $(f-1)$ freedoms.

3 Phase space SOS representation of quantum SOS states

For some purposes one would like to have as close correspondence with classical Poincaré dynamics as possible. The classical system can be efficiently described in terms of probability distribution function over the $2(f-1)$-dim SOS with coordinates $\boldsymbol{z} = (\boldsymbol{x}, \boldsymbol{p}_{\boldsymbol{x}})$. Classical Poincaré mapping τ_E on points $\boldsymbol{z}$ or distribution functions $f(\boldsymbol{z})$ can be written as

$$\boldsymbol{z}_{n+1} = \tau_E(\boldsymbol{z}_n), \tag{39}$$

$$f_{n+1}(\tau_E(\boldsymbol{z})) = f_n(\boldsymbol{z}). \tag{40}$$

Classical invariant distributions, fixed points of τ_E, are characteristic functions over disjoint classical invariant components of SOS which can be either periodic orbits, or $(f-1)$-dim invariant tori, or $2(f-1)$-dim chaotic regions. From the full space quantum mechanics we adopt coherent state representation for the quantum SOS distribution of an SOS state $|\psi\}$ and call it SOS Husimi distribution

$$\Psi^{\rm h}_\alpha(\boldsymbol{z}) = |\{\boldsymbol{z},\alpha|\psi\}|^2, \quad \{\boldsymbol{x}'|\boldsymbol{x},\boldsymbol{p}_{\boldsymbol{x}},\alpha\} = (2\pi\hbar\alpha)^{\frac{1-f}{4}} \exp\left(-\frac{(\boldsymbol{x}-\boldsymbol{x}')^2}{2\alpha\hbar} + \frac{i\boldsymbol{p}_{\boldsymbol{x}}\cdot\boldsymbol{x}'}{\hbar}\right), \tag{41}$$

which is not unique but depends on the deformation α of the minimal coherent states $|\boldsymbol{z},\alpha\}$. In completely similar way as for ordinary continuous time $(f-1)-dim$ quantum system one could also study the familiar Wigner [33] distribution but for the purposes of this paper I prefer Husimi distribution because it is positive unlike Wigner. According to most general and strongest correspondence principle, the so called *principle of uniform semiclassical condensation* [3, 29, 14], in the semiclassical limit $\hbar \to 0$ phase space distributions of quantum eigenstates as well as quantum states evolving for sufficiently long time should condense on classically invariant components. So SOS Husimi distribution $\Psi^{\mathrm{h}}_{\alpha}(\boldsymbol{z})$ of a typical eigenstate, where $|\psi\}$ is the corresponding fixed point of unitary QPM, should appear very much like classical plot of chaotic region or some regular invariant torus. In the next section we present numerous numerical results concerning the demonstration of this principle in a generic nonlinear dynamical system obtained by the quantum SOS method.

For quantitative analysis we define localization area (volume) of a given normalized SOS state $|\psi\}$ through its information entropy

$$A_{\psi} = c_{f-1} \exp\left(-\int dz \Psi^{\mathrm{h}}_{\alpha}(\boldsymbol{z}) \ln \Psi^{\mathrm{h}}_{\alpha}(\boldsymbol{z})\right) \tag{42}$$

The localization area A_{ψ} measures the effective area of SOS occupied by a state $|\psi\}$ i.e. the area where the SOS Husimi distribution is significant. c_{f-1} is some dimensionless normalization constant which may be determined by the requirement that Husimi function generated by truly *Gaussian random* wavefunction, the so called Gaussian Random Husimi distribution (GRHD), should have localization volume equal to the volume of entire classically allowed region of phase space, yielding numerically in 2-dim $c_1 \approx 1.538$. In order to get more information about the structure of SOS states one could use the concept of generalized entropies to define corresponding generalized localization areas $A_{\psi}(s)$ for $s > 0$

$$A_{\psi}(s) = c_{f-1}(s) \left[\int dz \left(\Psi^{\mathrm{h}}_{\alpha}(\boldsymbol{z})\right)^{1+s}\right]^{-1/s} \tag{43}$$

with the usual localization area as the limit $A_{\psi} = A_{\psi}(s \to +0)$. Again we may use GRHD to determine normalization constants $c_{f-1}(s)$. Here are some numerical values $c_1(1) \approx 2.02, c_1(2) \approx 2.49, c_1(3) \approx 2.94$.

4 Application of quantum SOS method to quantum chaos

In this section I will present the results of extensive numerical application of quantum SOS method to a generic 2-dim bound autonomous Hamiltonian system, namely the semi-separable oscillator. Due to efficiency of quantum SOS method which effectively reduces the labor by one degree of freedom and special geometric structure of our system we were able to reach extremely deep semiclassical regime, namely we were able to calculate thousands of consecutive levels with sequential quantum number around twenty million. Thus we are able to test various conjectures of quantum chaos about the structure of eigenstates and statistical properties of spectra.

4.1 The system and practical quantization technique

The most practical quantization condition of quantum SOS method is the singularity condition for the sum of Hermitian reactance operators (29)

$$\det \tilde{\mathbf{R}}(E) = 0, \tag{44}$$

which are for numerical calculations represented by finitely dimensional matrices $\tilde{\mathbf{R}}(E) = \tilde{\mathbf{R}}_{\uparrow}(E) + \tilde{\mathbf{R}}_{\downarrow}(E)$ in a truncated $(N = N_o + N_c)$-dim basis of $N_o = \dim \mathcal{L}_o(E)$ open modes and sufficiently large number N_c of first closed modes such that the zeros of (44) converge. Let $\Psi_{\sigma n}(\boldsymbol{x}, y, E)$ denote the two unique sets of solution of Schrödinger equation (2) on either $\sigma-$side $\mathcal{C}_\sigma$ and with boundary conditions $\Psi_{\sigma n}(\boldsymbol{x}, 0, E) = \{\boldsymbol{x}|n\}, \Psi_{\sigma n}(\boldsymbol{q} \in \mathcal{B}_\sigma, E) = 0$. In other words, $|\Psi_{\sigma n}(E)\rangle = \acute{W}_\sigma(E)|n\}$. For real energy E the matrix elements of Hermitian reactance matrices can be written as

$$\tilde{\mathbf{R}}_{\sigma nl}(E) = \{n|\check{\mathcal{R}}(E)|l\} = \frac{\sigma}{\sqrt{|k_n(E)k_l(E)|}} \int d\boldsymbol{x} \Psi^*_{\sigma n}(\boldsymbol{x}, y, E) \partial_y \Psi_{\sigma l}(\boldsymbol{x}, y, E)|_{\sigma y = +0}. \tag{45}$$

If the system possesses a *time-reversal* symmetry then the Hermitian reactance matrices $\tilde{\mathbf{R}}_\sigma$ are *real* (and *symmetric*) due to reality of wavefunctions $\Psi_{\sigma n}(\boldsymbol{q}, E)$ and therefore their Caley transforms, unitary conditional CSOS-CSOS propagators have *symmetric* matrices $\{n|\check{\mathcal{T}}_\sigma(E)|l\} = \{l|\check{\mathcal{T}}_\sigma(E)|n\}$.

Reactance matrices can be most easily calculated for the so-called *semiseparable* systems, that is, for systems which are separable (in $(\boldsymbol{x}, y)$ coordinates) on both sides of CS $\mathcal{C}_\sigma$ but they have possible discontinuity on CSOS so that they are not separable on the whole CS $\mathcal{C}$ [23].

One such semiseparable system which turned out to be very convenient for numerical work is the so-called $(f = 2)$-*dim semiseparable oscillator* (SSO) with the Hamiltonian

$$H(x, y, p_x, p_y) = \tfrac{1}{2}p_x^2 + \tfrac{1}{2}p_y^2 + \tfrac{1}{2}(x + \tfrac{1}{2}\mathrm{sign}(y)a)^2, \quad -b_\downarrow \le y \le b_\uparrow \tag{46}$$

The potential is harmonic in $x-$direction while it is flat with perfect hard walls at $y = -b_\downarrow, b_\uparrow$ in $y-$direction. The classical dynamics of SSO was also extensively studied and it was found that the system exhibits all the features of generic nonlinear softly chaotic 2-dim autonomous Hamiltonian systems. For limiting cases $a = 0$ (single box limit) and $a = \infty$ (two box limit) the system is integrable, while for most other values of parameters the system has mixed classical dynamics with regular and chaotic regions coexisting in phase space and on SOS $(x, p_x; y = 0)$, for some values of parameters the system is even fully chaotic – ergodic (see e.g. figure 5c). [3] The quantized SSO described by Hamilton operator $\hat{H} = H(x, y, -i\hbar\partial_x, -i\hbar\partial_y)$ has a 1-dim scaling symmetry $(a, b_\sigma, E) \to (\lambda a, \lambda b_\sigma, \lambda^2\hbar, \lambda^2 E)$. The reduced Hamiltonian is just a simple 1-dim harmonic oscillator $\check{H}' = -\frac{1}{2}\hbar^2\partial_x^2 + \frac{1}{2}x^2$ with *real* SOS eigenmodes

$$\{x|n\} = \{n|x\} = (\sqrt{\pi\hbar}2^n n!)^{-1/2} \exp(-x^2/2\hbar) H_n(x/\sqrt{\hbar})$$

and threshold energies $E'_n = (n + \frac{1}{2})\hbar$ determining the wavenumbers

$$k_n(E) = \hbar^{-1}\sqrt{2E - (2n+1)\hbar}, \quad n = 0, 1, 2 \ldots$$

[3] The ergodicity in such special cases has not been rigorously proved but it can be shown numerically that the total volume of regular components can be made unmeasurably small. For example, for any $0 < a < \sqrt{8E}$ the system becomes ergodic in the limit $b_\downarrow + b_\uparrow \to \infty$.

Due to separability the solutions of Schrödinger equation on each side $\mathcal{C}_\alpha$ are composed of products $\{x+\frac{1}{2}\sigma a|n\}\sin(k_n(E)(b_\sigma-\sigma y))/\sin(k_n(E)b_\sigma)$ but because of defect on CSOS at $y=0$ one should use unitary *shift operator* $\check{O}=\exp(ia\check{p}_x/2\hbar)$ with matrix elements

$$\mathbf{O}_{nl}=\int dx\{n+\tfrac{1}{2}a|x\}\{x|l\}$$

to generate SOS induced solutions

$$\Psi_{\sigma n}(x,y,E)=\sum_l\{x+\tfrac{1}{2}\sigma a|l\}\frac{\sin(k_l(E)(b_\uparrow-\sigma y))}{\sin(k_l(E)b_\uparrow)}\mathbf{O}_{\sigma ln}, \tag{47}$$

where we write $\mathbf{O}_{\uparrow nl}=\mathbf{O}_{nl}$, $\mathbf{O}_{\downarrow nl}=\mathbf{O}_{ln}$. So, using (45), *real symmetric* reactance matrices for SSO read

$$\tilde{\mathbf{R}}_{\sigma nl}(E)=-|k_n(E)k_l(E)|^{-1/2}\sum_j\mathbf{O}_{\sigma nj}k_j(E)\cot(k_j(E)b_\sigma)\mathbf{O}_{\sigma lj}. \tag{48}$$

The matrix elements of shift operator can be numerically calculated via stable symmetric recursion

$$\begin{aligned}\mathbf{O}_{n,0} &= (-1)^n\mathbf{O}_{0,n}=\frac{1}{\sqrt{n!}}\exp\left(-\frac{a^2}{16\hbar}\right),\\ \mathbf{O}_{n,l} &= \frac{n+l}{\sqrt{4nl}}\mathbf{O}_{n-1,l-1}-\frac{a}{\sqrt{32\hbar n}}\mathbf{O}_{n-1,l}+\frac{a}{\sqrt{32\hbar l}}\mathbf{O}_{n,l-1}.\end{aligned}$$

The number of open modes of SSO is $N_o=round(E/\hbar)$. In order to determine minimal number of closed modes N_c, such that the results are expected to converge one can use semiclassical arguments, namely, SOS phase space supports of coherent state representation of basic SOS states $|n\},0\le n\le N_o+N_c-1$ should cover the supports of first N_o shifted states $\check{O}|n\},0\le n\le N_o-1$

$$N_c=\left(\frac{2a}{\sqrt{2E}}+\frac{a^2}{2E}\right)N_o.$$

It is very important to stress that the shift matrix $\mathbf{O}_{nl}$ and therefore also the reactance matrices $\tilde{\mathbf{R}}_{\sigma nl}(E)$ are effectively banded, that is, their elements are decreasing exponentially fast when the distance from diagonal $|n-l|$ becomes larger than the effective bandwidth. One can again derive semiclassical formula for the effective bandwidths using overlap condition for the coherent state representation of the SOS states $|n\}$ and $\check{O}|l\}$

$$\text{bandwidth}(\tilde{\mathbf{R}}_\sigma(E))=2\text{bandwidth}(\mathbf{O})\approx\frac{2a}{\sqrt{2E}}N_o \tag{49}$$

Note that the function $f(E)=\det\tilde{\mathbf{R}}(E)$ has singularities (poles) at the points E where for some n, $k_n(E)b_\sigma$ is a multiple of π. But between the two successive poles $f(E)$ is smooth (even analytic) real function of real energy E. I have devised an algorithm for calculation of almost all levels — zeros of $f(E)$ within a given interval $[E_i,E_f]$ which needs to evaluate $f(E)$ which takes $\mathcal{O}(\text{bandwidth}^2N)$ FPO only about 25 times per mean level spacing while it typically misses less than 0.5% of all levels. The control over missed levels is in general a very difficult problem. The number of all energy levels below a given energy E, $\mathcal{N}(E)$ can be estimated by means of the Thomas-Fermi rule

$$\mathcal{N}(E)\approx\mathcal{N}^{\text{TF}}(E)=\frac{b_\uparrow+b_\downarrow}{3\pi\hbar^2}(2E)^{3/2}. \tag{50}$$

But this formula is generally not very helpful even if next semiclassical corrections are negligible since the fluctuation of the number of levels in an interval $[E_i, E_f]$ is proportional to $\sqrt{\mathcal{N}(E_f) - \mathcal{N}(E_i)}$ except in the extreme case of fully chaotic systems where the spectra are much stiffer and the fluctuation is proportional to $\log[\mathcal{N}(E_f) - \mathcal{N}(E_i)]$ so that Thomas-Fermi rule can be used to detect even single missing level [7, 1].

We have chosen the following values of parameters $a = 0.03, b_\downarrow = 5.0, b_\uparrow = 10, E = 0.5$, while for quantal calculations we take the energy to be in a narrow interval around $E = 0.5$. Careful examination of classical dynamics (for Poincaré SOS plot see figure 4w) showed that there is only one dominating chaotic component of phase space of relative volume $\rho_2 = 0.709 \pm 0.001$ (which is not equal to its relative SOS area) while regular component together with other very small chaotic components have total relative volume $\rho_1 = 1 - \rho_2 = 0.291 \pm 0.001$. We have calculated two stretches of consecutive energy levels and corresponding eigenstates: (case I) 14 231 levels in the interval $0.35 < E < 0.65$ for $\hbar = 0.01$ with sequential quantum number according to (50) equal to $\mathcal{N} \approx 16\,000$, (case II) and 13 445 levels in the interval $0.49985 < E < 0.500105$ for $\hbar = 0.0003$ with sequential quantum number $\mathcal{N} \approx 17\,684\,000$.

Large square root number fluctuations prevent to determine the number of missed levels by using Thomas-Fermi rule (although higher order semiclassical corrections are negligible in this regime). One can compare the number of levels $\mathcal{N}(E)$ with the number of levels $\mathcal{N}_0(E)$ or $\mathcal{N}_\infty(E)$ for the two nearby integrable – separable cases (with the same b_σ but with $a = 0$ (single box limit) or $a \to \infty$ (two box limit), respectively) since the leading order semiclassics (Thomas-Fermi rule) does not depend upon the defect a. $\mathcal{N}_0(E)$ and $\mathcal{N}_\infty(E)$ can be easily calculated numerically and *large scale* fluctuations of $\mathcal{N}(E) - \mathcal{N}_{0,\infty}(E)$ turn out to be much smaller than the fluctuations of $\mathcal{N}(E) - \mathcal{N}^{\mathrm{TF}}(E)$ suggesting that we have missed *less* than 20 levels out of 14 231 at $\hbar = 0.01$ and 40 - 80 levels out of 13 445 at $\hbar = 0.0003$. Note that in the first case ($\hbar = 0.01$) there was much less almost degenerate pairs of levels (and therefore less missed levels) due to the level repulsion.

For each zero of equation (44), eigenenergy E, one can determine the components $\rho_n = \{n|\rho\}$ of SOS representation $|\rho\}$ of the corresponding eigenstate by solving the homogeneous equation

$$\sum_l \tilde{\mathbf{R}}_{nl}(E)\rho_l = 0.$$

The corresponding eigenfunction $\Psi(\boldsymbol{x}, y)$ can be written as

$$\Psi(x, y) = \sum_l \frac{\rho_l}{\sqrt{|k_l(E)|}} \Psi_{\mathrm{sign}(y)l}(x, y, E) \tag{51}$$

where the wavefunctions $\Psi_{\sigma l}(x, y, E)$ are given by (47). For the SOS Husimi distribution of (eigen)states of SSO it seems natural choice to take coherent states with $\alpha = 1$ since basic SOS state $|0\}$ is then just a coherent state located at the origin $\boldsymbol{z} = (0, 0)$. In polar coordinates, $r = \sqrt{x^2 + p_x^2}, \phi = \arctan(p_x/x)$ the corresponding SOS Husimi function

$$\Psi^{\mathrm{h}}(\boldsymbol{z}) = |\{\boldsymbol{z}|\psi_\uparrow\}|^2 = \frac{1}{2\pi\hbar} \left| \sum_n \frac{u^n}{\sqrt{n!}} \psi_n e^{-in\phi} \right|^2 e^{-u^2}, \quad u = \frac{r}{\sqrt{2\hbar}} \tag{52}$$

can be efficiently calculated by means of Fast Fourier Transformation where $\psi_n = \{n|\psi_\uparrow\}$ are the components of the corresponding fixed point of the unitary QPM $|\psi_\uparrow\} = \frac{1}{2}(1 - i\check{\mathcal{R}}_\uparrow)|\rho\}$ (see eqs. (32,28),

$$\psi_n = \rho_n - i \sum_l \tilde{\mathbf{R}}_{\uparrow nl}(E)\rho_l.$$

4.2 Classification of eigenstates and Berry-Robnik level spacing distribution

According to principle of uniform semiclassical condensation the phase space distributions of eigenstates (such as Husimi) should uniformly condense on the classical invariant components of phase space, which may be either regular — tori, or chaotic, when $\hbar \to 0$. This condensation should be understood in a weak sense, i.e. quantum phase space distribution smoothed over many Planck's cells should approach characteristic function of a classical invariant component. Thus any quantum state, if $\hbar$ is sufficiently small, can be classified either as *regular* or *chaotic*, if it is associated with classically regular or chaotic component, respectively.

Berry and Robnik [4] also assumed that the energy levels of states associated with different disjoint classical components cannot be statistically correlated, so that the entire energy spectrum is a superposition of statistically uncorrelated level subsequences associated with different classical invariant components. The most characteristic is the so-called level spacing distribution $P(S)$, where $P(S)dS$ is a probability that a randomly chosen spacing between two adjacent energy levels lies between $S - dS/2$ and $S + dS/2$. All regular levels may be merged together giving a totally uncorrelated sequence with the so-called Poissonian statistics with $P_{\rm Poisson}(S) = e^{-S}$ while each chaotic subsequence is statistically equivalent to the spectrum of a fully chaotic system and therefore also [6] to the spectra of infinitely dimensional Gaussian orthogonal/unitary random matrices (GOE/GUE) provided that chaotic states are mainly delocalized – extended over the whole chaotic component. The gap distribution $E(S) = \int_S^\infty d\sigma(\sigma - S)P(\sigma)$ factorizes upon statistically independent superposition of spectra, so if one assumes only one practically dominating chaotic component with relative volume ρ_2 and regular and tiny chaotic components with total relative volume $\rho_1 = 1 - \rho_2$ the ultimate semiclassical Berry-Robnik formula reads

$$E^{\rm BR}_{\rho_1}(S) = E^{\rm Poisson}(\rho_1 S)E^{\rm GOE}(\rho_2 S), \quad P^{\rm BR}_{\rho_1}(E) = \frac{d^2}{dS^2}E^{\rm BR}_{\rho_1}(S). \tag{53}$$

This two component Berry-Robnik formula will apply also to SSO with $a = 0.03, b_\uparrow = 5, b_\downarrow = 10, E = 0.5$, where we have indeed only one large dominating chaotic region (see figure 4w). The Berry-Robnik distribution does not exhibit *level repulsion*, since $P^{\rm BR}_{\rho_1}(0) = 1 - \rho_2^2 \neq 0$. On the other hand there has been a vast amount of phenomenological evidence [28] in favour of the so called *fractional power law level repulsion* which is globally very well described by the Brody [8] distribution

$$P^B_\beta(S) = aS^\beta \exp(-bS^{\beta+1}), \quad a = (\beta+1)b,\ b = [\Gamma(1 + (\beta+1)^{-1})]^{\beta+1} \tag{54}$$

which is characterized by the noninteger exponent β, $P(S \to 0) \propto S^\beta$. Numerical spectra which contain even up to several ten thousands energy levels of quantum Hamiltonian systems with mixed classical dynamics typically still exhibit the phenomenon of fractional level repulsion, with statistically significant global fit by the Brody distribution. In such cases there was a persisting puzzle as for how the level spacing distribution converges to the semiclassical Berry-Robnik distribution as one increases the sequential quantum number or decreases the value of effective $\hbar$. However, recently we have succeeded to demonstrate the ultimate semiclassical Berry-Robnik level spacing distribution in a rather abstract 1-dim time-dependent dynamical system, namely the standard map on a torus, and showed (smooth) transition from Brody-like to Berry-Robnik distribution

as $\hbar$ decreases [27, 28] (see also [21]), and more recently the first such demonstration in a generic 2-dim autonomous conservative system is provided by the SSO [24].

Let us estimate the maximal (critical) value of the effective Planck's constant $\hbar_{\max}$ of the far semiclassical regime where Berry-Robnik approach is expected to be valid. There are two conditions to be satisfied:

- States which live on classically disjoint invariant components should have small overlap to provide statistical independence of partial subspectra. Husimi phase space distributions of quantum (chaotic or regular) eigenstates typically decay like Gaussian into classically forbidden neighbouring (regular or chaotic) invariant region with an effective penetration depth equal to $\sqrt{\hbar}$ (see e.g. [33]). It seems reasonable to require that this quantum resolution scale should be much smaller than dimensions of classical chaotic region, say at least 10 times smaller than the radius $r_{\rm C}$ of the largest ball which lies entirely in the chaotic component of SOS, $\sqrt{\hbar} \lesssim 0.1 r_{\rm C}$. For SSO with $a = 0.03, b_\uparrow = 5, b_\downarrow = 10$ we have $r_{\rm C} \approx 0.16$ (see figure 4w), so $\hbar \lesssim 0.0003$.

- Chaotic states should be delocalized – extended over the whole classical chaotic region of phase space in order to justify usage of maximal entropy ensembles of random matrices (GOE/GUE) to model chaotic subspectra. If μ_2 is a relative area of chaotic component of SOS then SOS Husimi distributions of last $\mu_2 N_o$ open SOS eigenmodes $|n\}$ (thin circular rings in case of SSO) approximately support the chaotic region (which has the shape of a ring in case of SSO (see figure 4w)). Quite generally [25] QPM is represented by a banded matrix (having approximately independent $\mu_2 N_o$-dim chaotic block) with a minimal bandwidth $b \approx 4a\mu_2 N_o/\sqrt{2\mu_2 E}$ in case of SSO. Using the theory of localization of eigenvectors in finite banded random matrices [9, 12] one can write the condition for, say 90% delocalization of chaotic states of SSO $1.4\frac{b^2}{\mu_2 N_o} \gtrsim \frac{0.9}{1-0.9}$, giving

$$\hbar \lesssim a^2. \tag{55}$$

  For SSO with $a = 0.03$ we have the condition $\hbar \lesssim 0.0009$.

The far semiclassical regime sets in if

$$\hbar \lesssim \hbar_{\max} = \min(0.01 r_{\rm C}^2, a^2)$$

and the case II has been chosen to optimally meet this condition.

Unique classification of states into regular and chaotic class is a necessary condition for the validity of Berry-Robnik formula and it can be performed quantitatively as follows. Let us define a *probability distribution of localization areas* $\mathcal{P}(A)$ where $\mathcal{P}(A)dA$ is a probability that a randomly chosen eigenstate have SOS localization area (42) between $A - dA/2$ and $A + dA/2$. For two component case with a single dominating chaotic region $\mathcal{P}(A)$ is expected to be bimodal, one sharp peak of width proportional to $\mathcal{O}\left(\hbar^{\frac{f-1}{2}}\right)$ close to $A = 0$ correspond to regular states while the other, wider peak located at SOS area of chaotic component correspond to chaotic states. The width of the second peak is a more complicated and yet unsolved function of $\hbar$ and geometry. Find the area $A_{\min}$ between the two peaks where $\mathcal{P}(A)$ takes its minimum. A quantum state with SOS localization

area A is said to be *regular* if $A < A_{\min}$ and *chaotic* if $A > A_{\min}$. The integrated probability for a randomly chosen state to be regular should match with the relative volume of classical regular component

$$\rho_1^A = \int_0^{A_{\min}} dA\mathcal{P}(A) \tag{56}$$

This was nicely confirmed for the stretch of 14 thousand eigenstates of *far* semiclassical case II ($\hbar = 0.0003$), giving $\rho_1^A = 0.293 \pm 0.004$ in excellent agreement with the classical value $\rho_1 = 0.291$ (see figure 1a), whereas for the *near* semiclassical case I ($\hbar = 0.01$) the localization area distribution $\mathcal{P}(A)$ was still unimodal, indicating that eigenstates cannot be clearly and uniquely classified as regular or chaotic (figure 2a).

The level spacing statistics behaves in complete agreement with the results of this classification. For case II one obtains significant fit ($\chi^2 = 12150$) with Berry-Robnik distribution (53) (figure 3b). I have also separated the entire spectrum into regular and irregular part according to classification in terms of localization area statistics and studied level spacing distribution for each part separately. The statistics of the regular part which contains 3791 levels, is indeed very close to Poissonian (figure 3c). The statistically significant fit with Berry-Robnik distribution gives $\rho_1 = 0.86, \chi^2 = 1500$ while fit with Brody distribution gives $\beta = 0.006, \chi^2 = 2300$. The statistics of the irregular part, which contains 9652 levels, is slightly further from but still close to GOE (figure 3d). The Berry-Robnik fit is only slightly nonsignificant, $\rho_1 = 0.04, \chi^2 = 15000$, while Brody fit is worse, giving $\beta = 0.83, \chi^2 = 23000$. These results (figure 3) clearly confirm Berry-Robnik picture (which is claimed to be an asymptotically — as $\hbar \to 0$ — exact theory [26, 27, 28]) although we still see small but still significant deviations from the expected statistics of partial spectra, because of small but still existing correlations between regular and irregular levels due to (small) overlap of corresponding eigenstates, and because of localization of some irregular states on small subregions of chaotic orbit where classical dynamics is almost trapped, such as near chaos border (see also figures 4i,4t)). On the other hand, energy level spacing distribution of the near semiclassical case I still exhibits power law level repulsion with statistically significant fit by Brody distribution (54) with $\beta = 0.142, \chi^2 = 5320$ (figure 3a).

There is another useful quantitative measure of a given SOS state $|\psi\}$, namely, *quantum-classical overlap*: the overlap between SOS Husimi distribution and the classical chaotic component $\mathcal{S}_C$ of SOS

$$B_\psi = \int_{\mathcal{S}_C} d\boldsymbol{z}\Psi^\alpha(\boldsymbol{z}). \tag{57}$$

The state $|\psi\}$ is irregular if B_ψ is close to 1 and regular if B_ψ is significantly less than 1. Similar classification has been recently performed in a Robnik billiard [15]. Again we define the probability distribution of quantum-classical overlaps $\mathcal{P}(B)$: $\mathcal{P}(B)dB$ is a probability that the quantum-classical overlap of a randomly chosen state lies between $B - dB/2$ and $B + dB/2$. We expect and confirm (figures 1 and 2) that this distribution has qualitatively the same properties (bimodality) with even sharper peaks as localization area distribution $\mathcal{P}(A)$. $\mathcal{P}(B)$ is bimodal even for the case I and thus provides a measure for classification of states for near semiclassical regime where localization area statistics fails. But for far semiclassical regime (case II) the $\mathcal{P}(A)$ has lower minimum than $\mathcal{P}(B)$ and thus provide clearer classification of eigenstates. The scatter diagram (figures 1f,2f) A_ψ versus B_ψ is very interesting and helps us to discover states with some special or exotic geometry, e.g. the regular states which live on small regular islands inside chaotic

region (see figure 4(g,h,r,s,w)). These states have small localization area A whereas their quantum-classical overlap B is significantly different from zero while for all other regular states living in the large central island B is extremely close to zero.

4.3 Gallery of eigenstates

For the systems of two freedoms ($f = 2$) SOS Husimi distributions provide certainly the most elegant and efficient way of graphical presentation of quantum eigenstates. In figure 4 I present the SOS Husimi distributions of eleven eigenstates of far semiclassical case II. The first six of them are typical consecutive states within the qualitative conclusions of previous subsection: the two regular states are strongly localized over corresponding tori, while three out of four chaotic states are very much uniform over the chaotic component with lots of (GRHD-like) microscopic structure which is responsible for the normalization factor $c_1 = 1.54$ in the definition of localization area (42). The fourth chaotic state (figures 4(e,p)), which is rather exceptional in this regime, is mainly localized only in the outer part of chaotic component due to circular partial classical barrier at $r \approx 0.81$ [7]. The remaining five states are the specially picked states which have geometrically extremal properties: (i) the regular states with smallest area and smallest quantum-classical overlap on the small regular islands inside chaotic component (figures 4(g,h,r,s)), (ii) the chaotic state which is strongly localized around the chaos border where the classical dynamics is almost trapped (figures 4(i,t)), (iii) the mixed state which is almost uniformly localized over chaotic component and a torus which is geometrically close to chaotic component (figures 4(j,u)), and (iv) a chaotic state which lives on a small broken separatrix (figures 4(k,v)). We always give two graphical representations of SOS Husimi distributions: *equidistant contour plot* with ten contours separated by 1/10 of the maximal value of SOS Husimi distribution starting with 1/20 of the maximum, and logarithmic five contour plot where neighbouring contours are by a constant factor of $\hbar^{-0.2}$ apart (the values of SOS Husimi distribution at the first and last contour differ by a factor of $1/\hbar$). The two presentations are complementary: equidistant plot shows only the most important features of an eigenstate whereas logarithmic plot slightly obscures the most important features and shows also the important details of SOS Husimi distribution such as extension over classical invariant components or distribution of its zeros.

I have also calculated a sequence of 16 consecutive eigenstates in a classically fully chaotic — practically ergodic regime $a = 0.25, b_\uparrow = 4, b_\downarrow = 11, \hbar = 0.0003, 0.49999 \leq E \leq 0.4999903$ (case III). The sequential quantum number is here the same as for case II, $\mathcal{N} \approx 17\,684\,000$. SOS Husimi functions of all 16 states were very uniformly extended over the whole classically allowed region of SOS which confirm one of the basic conjectures of quantum chaos (see figure 5) [3].

In figure 6 I show the CS wavefunctions of two typical eigenstates of case II, a regular and a chaotic, which were calculated according to formula (51). Despite extremely high sequential quantum numbers the chaotic wavefunctions are globally scarred with many (stretches of) classical orbits, whereas on smaller scales they appear much more Gaussian random. On the other hand, wavefunctions of fully chaotic case III appear uniformly random (without any structure) even on the largest scale (an example is given in figure 7).

In order to test numerical method and to search for possible large scale nonuniformi-

ties in wavefunctions I have defined also a *contrast* of a wavefunction $\Psi(x,y)$ by

$$C_\psi = \frac{\int dx \int_{-b_\downarrow}^{b_\uparrow} dy \left(\frac{\theta(y)}{b_\uparrow} - \frac{\theta(-y)}{b_\downarrow}\right) |\Psi(x,y)|^2}{\int dx \int_{-b_\downarrow}^{b_\uparrow} dy \left(\frac{\theta(y)}{b_\uparrow} + \frac{\theta(-y)}{b_\downarrow}\right) |\Psi(x,y)|^2}. \tag{58}$$

Again, $\theta(y)$ is the Heaviside step function. The contrast C_ψ lies between -1 and $+1$ and measures the difference between quantum and classical probability that the system lies above or below CSOS. I have also studied the probability distribution of contrasts $\mathcal{P}(C)$ for cases I and II (figures 1c,2c): $\mathcal{P}(C)dC$ is a probability that randomly chosen eigenstate has a contrast between $C - dC/2$ and $C + dC/2$. Contrast may be used to detect scars of periodic orbits. I found that large majority of eigenstates has a contrast very close to zero. But contrast may be significantly different from zero for some *chaotic* states, since contrast C_ψ is strongly correlated with localization area A_ψ and especially with quantum-classical overlap B_ψ (see scatter diagrams 1(d,e),2(d,e)). These states must be scarred by classical periodic orbits since these are typically not balanced with respect to CSOS. It has been numerically checked and found that by far most frequent are the so called bouncing-ball-like scars, which can have the largest contrast (up to 1), and which are associated with a continuous family of neutrally stable orbits with $y = \text{const}$. I show one example for case II in figure 8.

4.4 Distribution of zeros of SOS Husimi distribution

According to Bargmann [2] the 2-dim Husimi distributions of quantum states may generally be written as $|f(x+ip_x)|^2 \exp(-(x^2+p_x^2)/2\hbar)$ where f is a complex analytic function. This is indeed the case for SSO (52). The zeros of SOS Husimi distributions are thus simple points in SOS and their distribution can be associated with the dynamical properties of an underlying system [17]. The zeros of SOS Husimi distributions of chaotic states are expected and confirmed to be uniformly distributed over the chaotic component of SOS (figure 9, especially if the system is fully chaotic (figure 10) [17]). SOS Husimi distribution of a chaotic eigenstate in a generic mixed system have also zeros on the regular component where the zeros condense on the regular invariant curves — tori (see figure 9). The large number of the zeros of regular states in a mixed system lies on some curves which are not classically invariant and which can even extend to chaotic region (generalization of anti-Stokes lines from [17]) while substantial number of zeros are also uniformly distributed over chaotic region and along regular invariant curves. But zeros for a regular state typically strongly avoid the classically invariant region of strongest localization of Husimi distribution (figure 9(a,d,g,h,j,k)). Even chaotic states of a fully chaotic system can have (1-dim-like) clusters of zeros lying outside classically allowed region of phase space (see figure 10).

So far there are no analytical or numerical results about other statistical measures of zeros of Husimi distribution of a chaotic state inside chaotic region, such as e.g. *nearest zero spacing distribution* $\mathcal{Z}(S)$: $\mathcal{Z}(S)dS$ is a probability that a distance between a randomly chosen zero and its nearest neighbour lies between $S - dS/2$ and $S + dS/2$. I have found numerically: (i) that zeros of SOS Husimi distribution which live in the chaotic region for $f = 2$ feel a cubic repulsion $\mathcal{Z}(S \to 0) \propto Z^3$ (figures 11,12), and (ii) the nearest zero spacing distribution for chaotic regions of chaotic states can be very well modeled by GRHD (the same as used to define the normalization c_f of localization areas) (figures 11,12), except for large spacings S it seems (see figures 11b,12b) that $\mathcal{Z}(S)$ behaves like $\ln \mathcal{Z}(S) \propto -Z^4$ while GRHD model suggests a Gaussian behaviour

$\mathcal{Z}(S) \propto -Z^2$. Further numerical and if possible analytical work is required to clarify and explain these observations.

4.5 Demonstration of Quantum Poincaré evolution

The physical motivation for an explicit study of quantum Poincaré time evolution in SSO is a quantum-classical correspondence: How long can a quantum evolution follow classical evolution? In order to explore this question is some detail we study a quantum Poincaré evolution of initial wave packet — coherent state $|\boldsymbol{z}\} = |\boldsymbol{z}, \alpha = 1\}$, $\boldsymbol{z} = (x, p_x)$ at fixed energy E in SOS Husimi representation

$$h_n(\boldsymbol{z}_f, \boldsymbol{z}_i, E) = |\{\boldsymbol{z}_f|\check{\mathcal{T}}^n(E)|\boldsymbol{z}_i\}|^2. \tag{59}$$

Classically, we should take the same initial wave packet SOS phase space distribution $|\{\boldsymbol{z}|\boldsymbol{z}_i\}|^2$, then classically evolve it (40), and finally take the classical probability that the system finds itself described by the final wave packet distribution $|\{\boldsymbol{z}|\boldsymbol{z}_f\}|^2$

$$f_n(\boldsymbol{z}_f, \boldsymbol{z}_i, E) = \int d\boldsymbol{z} |\{\boldsymbol{z}_f|\boldsymbol{z}\}|^2 |\{\tau_E^n(\boldsymbol{z})|\boldsymbol{z}_i\}|^2. \tag{60}$$

Such smoothed classical evolution of a wave packet $f_n(\boldsymbol{z}_f, \boldsymbol{z}_i, E)$, which is sometimes called *coarse-grained* classical dynamics [33], is a purely classical (not semiclassical) object which is expected to be most faithfully followed by the *quantum SOS phase-space propagator* $h_n(\boldsymbol{z}_f, \boldsymbol{z}_i, E)$. I plot these quantum and classical SOS phase space distributions for initial wave packet located somewhere in chaotic region for far semiclassical case II (figure 13) and near semiclassical case I (figure 14). In agreement with the results of stationary quantum mechanics we find, that in case II quantum dynamics explores the whole classically accessible part of SOS (the chaotic component) while in case I it remains localized on much smaller subregions of chaotic component. There exists a kind of *break iteration* $n_{\rm break}$ up to which quantum dynamics faithfully follows classical dynamics [10]. We can characterize this quantitatively by means of localization areas $A_n^{\rm q}, A_n^{\rm cl}$ of quantum and classical SOS distributions, h_n, f_n, respectively. (Note that for calculation of localization area of classical SOS distribution one should take $c_f = 1$ in formula (42).) So, for $n > n_{\rm break}$, $A_n^{\rm q}$ become significantly smaller than $A_n^{\rm cl}$. But $A_n^{\rm q}$ may still be increasing for $n > n_{\rm break}$ up to some $n_{\rm satur}$ where it saturates and then fluctuates around some average value $A_\infty^{\rm q}$. The far semiclassical regime, where the ultimate semiclassical formulas of quantum chaos (e.g. for level spacing distribution [4], for delta statistics [32], or for the statistics of matrix elements [20, 21]) are expected to hold, can be defined by the condition that arbitrary initial wave packet should explore the whole classically accessible region of phase space, i.e.

$$A_\infty^{\rm q} = A_\infty^{\rm cl}.$$

This is equivalent to the condition that eigenvectors of QPM $\check{\mathcal{T}}(E)$ *should not be localized* inside classically invariant chaotic components of SOS (55). In the opposite case QPM evolution of initial wave packet takes place only in the more or less small subspace spanned by these eigenvectors of QPM which have significant overlap with initial state. This is due to quantum localization [9, 12] which is a consequence of bandedness of QPM. Sufficient condition for the far semiclassical regime is that classical SOS distribution should reach an equilibrium within $n_{\rm break}$ iterations, $A_{n_{\rm break}}^{\rm cl} \approx A_\infty^{\rm cl}$.

To demonstrate these phenomena most clearly I have studied (in figure 15) the SOS dynamics of SSO in the so called *diffusively ergodic* regime of small $a \ll 1$ and very large $b_\uparrow + b_\downarrow \gg 1$ where classical dynamics is ergodic although it explores the accessible phase space rather slowly, with $r^2 = x^2 + p_x^2$ being an approximate second integral of motion. For $a = 0.03, b_\uparrow = 500, b_\downarrow = 1000$ the classical dynamics equilibrate after several hundred iterations while quantum dynamics quantitatively catches it only if $\hbar < 3 \cdot 10^{-4}$ or $N > 2 \cdot 10^3$ whereas 90% delocalization is achieved already for $\hbar = 0.0009$ (55) (between figures 15d and 15e).

5 Summary and conclusions

In the present paper I have introduced exact unitary quantum Poincaré mapping which has all the necessary properties: (i) it yields an exact and practically extremely useful quantization condition, and (ii) it can be literally interpreted as quantum CSOS-CSOS propagator since it is unitary and since energy dependent quantum propagator (Green function of the Schrödinger equation) can be decomposed in terms of CSOS-CSOS propagator and additional three conditional propagators between CS and CSOS which have been defined in the paper. In the second part of the paper I have applied this quantum SOS method for quantizing a simple but generic 2-dim autonomous Hamiltonian system, namely the semiseparable oscillator. I have studied both stationary and time evolving (better: SOS evolving) quantum dynamics of the system. Due to extreme efficiency of the method, especially for the so-called semiseparable systems, I have been able to go orders of magnitude higher than has previously been possible by any other method, up to 20 millionth eigenstate. Even for geometrically completely generic systems, such as e.g. diamagnetic Kepler problem [13], the method is expected to reach a millionth eigenstate [25]. I have confirmed Berry-Robnik scenario for level spacing distribution, classification of states into regular and irregular class, showed few typical and atypical examples of SOS Husimi distributions and wavefunctions of eigenstates, analyzed the distribution of zeros of SOS Husimi distributions of eigenstates and found uniformity with cubic nearest neighbour repulsion, and successfully compared quantum and classical Poincaré SOS evolution.

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Figures

Figure 1 Localization area distribution $\mathcal{P}(A)$ (a), Quantum-classical overlap distribution $\mathcal{P}(B)$ (b) and contrast distribution $\mathcal{P}(C)$ (c) for the 13445 eigenstates of SSO for $a = 0.03, b_\uparrow = 5, b_\downarrow = 10, \hbar = 0.0003$ (case II). The dark, black curves denote the cumulative (integrated) distributions, whereas bright, grey curves denote the usual probability densities. The thin black curve in (a) denote the cumulative distribution of generalized localization areas $A_\psi(1)$ which is much less sensitive and therefore less appropriate for the classification of eigenstates than the usual localization area distribution (thick black curve). The horizontal dotted lines in (a,b) denote the relative volume of classical regular component $\rho_1 = 0.291$ and vertical dotted lines in (a) denote the positions of maxima and minima of probability distributions. Scatter diagrams for the corresponding three quantities A_ψ, B_ψ, C_ψ are also shown: A_ψ vs. B_ψ (f), A_ψ vs. C_ψ (d), and B_ψ vs. C_ψ (e). Note the two tongues in scatter diagram (f) at small A and at $b \approx 0.17, 0.47$ correspond the regular states (e.g figure 4(g,r),4(h,s)) which live on small islands inside chaotic region (figure 4w) and have therefore significant overlap with the chaotic region.

Figure 2 Same as in figure 1 but for 14231 eigenstates of case I of SSO, $a = 0.03, b_\uparrow = 5, b_\downarrow = 10, \hbar = 0.01$. Although $P(A)$ (a) is here still unimodal, $P(B)$ is already bimodal and can be used for classification of eigenstates with threshold value of B selected at the point where the second (chaotic) peak starts and not at the minimum of probability density.

Figure 3 Cumulative energy level spacing distributions $W(S) = \int_0^S ds P(s)$ for the two cases of SSO for $a = 0.03, b_\uparrow = 5, b_\downarrow = 10$. The thick full curve are the numerical data, the thin full curve is the best-fit Berry-Robnik distribution, the dashed curve is the best-fit Brody distribution, and the dotted curves are the limiting Poisson and GOE distributions. For 14231 numerical energy levels of case I (a) $\hbar = 0.01$ one obtains significant global fit with Brody distribution, yielding the level repulsion exponent $\beta = 0.142$. For 13445 levels in the far semiclassical regime of case II (b) $\hbar = 0.0003$ we already obtain significant fit by the Berry-Robnik distribution with very accurate value of $\rho_1 = 0.283$. In (c) I show the cumulative level spacing distribution for regular part of the spectrum of case II which is indeed very close to Poisson, and (d) for irregular part of the spectrum which is also close to GOE (see text for details).

Figure 4 The figure shows SOS Husimi distributions of six typical eigenstates (above the dashed line: a-f,l-q) and five specially picked eigenstates with rare geometric properties (below the dashed line: g-k, r-v) for the far semiclassical case II of SSO: $a = 0.03, b_\uparrow = 5, b_\downarrow = 10, \hbar = 0.0003$. In figures (a-k) they are plotted with ten equidistant contours while in figures (l-v) they are plotted in logarithmic scale with five contours separating regions with different level of greyness, where each two neighbouring contours lie by a factor of $\hbar^{-0.2} = 5.06$ apart. The sequential numbers of the eigenstates states are around 17 684 000 with the following values of the eigenenergies: 0.49999967469 (a,l), 0.49999969040 (b,m), 0.49999970456 (c,n), 0.49999971683 (d,o), 0.49999974837 (e,p), 0.49999977984 (f,q), 0.50003435571 (g,r), 0.50000040776 (h,s), 0.49989001264 (i,t), 0.49996272064 (j,u), 0.49993911720 (k,v). I also give the few (two chaotic and two regular) classical SOS orbits in the same scale (w).

Figure 5 SOS Husimi distribution of a typical chaotic eigenstate with eigenenergy $E = 0.49999026441$ state in a *fully chaotic — ergodic* regime of SSO (case III: $a = 0.25, b_\downarrow = 4, b_\uparrow = 11, \hbar = 0.0003$). Equidistant (a) and logarithmic (b) contour plots have the same parameters as in figure 4. A single overwhelming classical chaotic orbit in SOS of the same scale is shown in (c).

Figure 6 Wavefunctions of a typical chaotic (a) and a regular (b) eigenstate of SSO with sequential quantum numbers around 17 684 000 (case II: $a = 0.03, b_\downarrow = 5, b_\uparrow = 10, \hbar = 0.0003$). Their SOS Husimi distributions are shown in figure 4(c,n) for (a) and in figure 4(d,o) for (b). In the left part of each figure the wavefunction in the entire configuration space $-1.025 \leq x \leq 1.025, -10 \leq y \leq 5$ is given with two black windows being magnified by a factor of 100 on the upper right side of the figure, in the same left-right order, and again with two black windows being magnified by another factor of 100 below, on the lower right side of the each figure. The regions where the magnitude of a square of the wavefunction (or its average over several tens de Broglie's wavelengths for the left part of each figure where the quantum resolution exceeds graphical resolution) is above suitably chosen threshold are painted black whereas everything else is white. SOS is indicated with a horizontal thin line.

Figure 7 The wavefunction of a typical chaotic eigenstate with sequential number around 17 684 000 and eigenenergy $E = 0.4999026441$ (its SOS Husimi distribution is shown in figure 5) in a *fully chaotic — ergodic* regime of SSO (case III: $a = 0.25, b_\downarrow = 4, b_\uparrow = 11, \hbar = 0.0003$). Presentational technique is the same as for figure 6 except for slightly extended region of $x-$coordinate on the left part $-1.15 \leq x \leq 1.15$ due to larger defect.

Figure 8 The wavefunction of a strongly (bouncing-ball-like) scarred chaotic eigenstate with sequential number around 17 684 000 and with eigenenergy $E = 0.4999999035$ (which is indeed very close (within mean level spacing) to quantization of a lower box with 106 nodes in $y-$direction which gives $E = 0.4999999027$) of SSO for case II: $a = 0.03, b_\downarrow = 5, b_\uparrow = 10, \hbar = 0.0003$. Presentational technique is the same as for figure 6.

Figure 9 The zeros of the SOS Husimi distributions are plotted for the same eleven eigenstates of SSO in the same scale as in figure 4. The edge of the largest chaotic region is marked with a thin curve so that one can easily observe the correlation between distribution of zeros and structure of classical SOS. Note the random uniform distribution of zeros on the chaotic component and regular distribution of zeros along regular classical invariant curves. Note also how zeros avoid regions of maximal Husimi density for regular states (a,d,g,h,j) and also for tiny chaotic state (k).

Figure 10 The zeros of the SOS Husimi distribution for the same typical chaotic eigenstate in ergodic regime of SSO as in figure 5 is shown in (a). The superposition of all (cca. 34800) zeros of 16 consecutive eigenstates which includes (a) is shown in (b) to demonstrate the uniformity of their distribution. For more quantitative conclusions I show also (c) the radial density of zeros (in arbitrary units) as determined from the zeros of these 16 eigenstates (b).

Figure 11 The cumulative nearest zero spacing distribution (a) $W(S) = \int_0^S ds \mathcal{Z}(s)$ is shown for cca. 16000 "chaotic" zeros of SOS Husimi distributions of 19 chaotic eigenstates from the sequence of 24 consecutive eigenstates for SSO of case II: $a = 0.03, b_\uparrow =$

$5, b_\downarrow = 10, \hbar = 0.0003, 0.4999995 \leq E \leq 0.5$ I have also plotted the corresponding T-function [26] $T(\ln S) = \ln(-\ln(1 - W(S)))$ to analyze behaviour at small and large spacings S where T-function is linear for power law S^β and exponential of a power $\exp(-S^\gamma)$, respectively. The numerical curve (thick curve (a), ±sigma statistical error bars (b)) excellently agrees with results obtained from statistical ensemble of GRHD (thin curves). The small S and large S parts are magnified in right-lower and left-upper window, respectively (a). Dashed line with a slope 4 is a guide for the eye (b) indicating that there is a cubic repulsion of zeros at small S.

Figure 12 The cumulative nearest zero spacing distribution (a) $W(S) = \int_0^S ds\mathcal{Z}(s)$ is shown for the zeros of SOS Husimi distributions of 16 chaotic states of SSO in the chaotic regime (the same eigenstates as in figure 10). Everything else is the same as in figure 11 including conclusions.

Figure 13 Quantum Poincaré phase space SOS time evolution $h_n(\boldsymbol{z}_f, \boldsymbol{z}_i, E)$ of an initial wave packet located at $x_i = 0, p_{xi} = 0.77$ is shown (with equidistant contours: a-f, and logarithmic contours: g-l with the same parameters as in figure 4) and compared with the corresponding coarse grained classical dynamics $f_n(\boldsymbol{z}_f, \boldsymbol{z}_i, E)$ (equidistant: m-q, logarithmic: r-v) for the far semiclassical regime of SSO (case II: $a = 0.03, b_\uparrow = 5, b_\downarrow = 10, \hbar = 0.0003, E = 0.5$). 1st (a,g while identical classical initial conditions are not plotted), 2nd (b,h,m,r), 3rd (c,i,n,s), 10th (d,j,o,t), 100th (e,k,p,u), and 1000th (f,l,q,v) iteration are shown. Note that both, quantum and classical state uniformly condenses on the classical invariant chaotic component.

Figure 14 The same as in figure 13 except for near semiclassical case I of SSO: $a = 0.03, b_\uparrow = 5, b_\downarrow = 10, \hbar = 0.01, E = 0.5$ and for 1st,2nd,3rd,5th,10th, and 100th iteration of Quantum Poincaré mapping. The quantum state does not condense on the entire classical invariant chaotic component of SOS but it remains localized on much smaller region of phase space (see figure 15). This phenomenon of quantum localization (in autonomous systems) is responsible for fractional power law level repulsion laws (see figure 3a).

Figure 15 The figure shows localization areas of quantum states which evolve under unitary quantum Poincaré mapping for the SSO in a diffusively ergodic regime $a = 0.03, b_\uparrow = 500, b_\downarrow = 1000, E = 0.5$ but for eight different values of effective Planck's constant: 0.0003 (a), 0.000424 (b), 0.0006 (c), 0.000849 (d), 0.0012 (e), 0.0017 (f), 0.0024 (g), 0.00339 (h) which increase geometrically by a factor of $\sqrt{2}$. The initial state is always a wave packet located at $x_i = 0, p_{xi} = 0.5$. The thick noisy curves denote localization areas of quantal states versus the number of iterations while the thick dotted curves denote localization areas of coarse grained classical states which evolve under classical Poincaré mapping. Note the very good agreement between the two curves up to some *break iteration*, where the two curves separate due to quantum localization except in the far semiclassical regime (a). The thin (full and dotted) curves denote the same quantities but on 10 times smaller iteration scale (up to 33rd iteration).